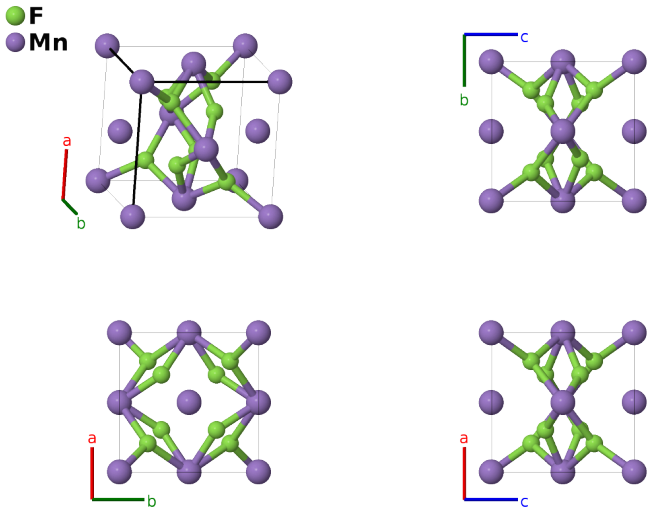
MnF_2 Structure: A2B_tP12_111_2n_bce-001

This structure originally had the label `A2B_tP12_111_2n_adf`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/YKCX

https://aflow.org/p/A2B_tP12_111_2n_bce-001

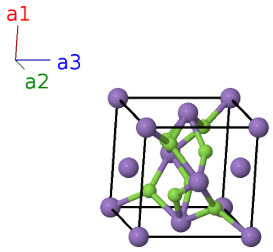


Prototype	F_2Mn
AFLOW prototype label	A2B_tP12_111_2n_bce-001
ICSD	12167
Pearson symbol	tP12
Space group number	111
Space group symbol	$P\bar{4}2m$
AFLOW prototype command	`aflow --proto=A2B_tP12_111_2n_bce-001 --params=`$a, c/a, x_4, z_4, x_5, z_5$

- This is the high pressure phase of MnF_2, with data taken at 200°C and 35 kbar. At standard temperature and pressure MnF_2 is in the rutile ($C4$) structure.
- (Yagi, 1979) consistently refers to space group $P\bar{4}2m$ as "#113," but it is actually #111, and the Wyckoff positions are consistent with $P\bar{4}2m$ #111.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Mn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1c)	Mn II
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2e)	Mn III
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(2e)	Mn III
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4n)	F I
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4n)	F I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4n)	F I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4n)	F I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4n)	F II
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4n)	F II
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4n)	F II
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4n)	F II

References

[1] T. Yagi, *Polymorphism in MnF_2 (rutile type) at high pressures*, J. Geophys. Res. **84**, 1113–1115 (1979), doi:10.1029/JB084iB03p01113.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.